U   Kell, Douglas B.; Goodacre, Royston; Neal, Mark J.
S   Institute of Biological Sciences, University of Wales, Aberystwyth, SY23
    3DA, UK
O   Proceedings of the ERDEC Scientific Conference on Chemical and Biological
    Defense Research, Aberdeen Proving Ground, Md., Nov. 14-17, 1995 (1996),
    Meeting Date 1995, 183-189. Editor(s): Berg, Dorothy A. Publisher:
    National Technical Information Service, Springfield, Va.
    CODEN: 64OYA8
T   Conference
A   English

> s specimen? and l15
      264666 SPECIMEN?
16   1 SPECIMEN? AND L15

> d

L16 ANSWER 1 OF 1 CA COPYRIGHT 2004 ACS on STN
N   128:50824 CA
I   Application of laser microprobe inductively coupled plasma mass
    spectrometry for trace metal **fingerprinting** of native gold
U   Chen, Zhongxing; Doherty, Will; Gregoire, D. Conrad; Harris, Don
S   Dept. of Geology, Mineral Resources Division, University of Windsor,
    Windsor, ON, N9B 3P4, Can.
O   Current Research - Geological Survey of Canada (1997), (1997-D), 57-62
    CODEN: CRGCED; ISSN: 0704-2884
PB Geological Survey of Canada
T   Journal
A   English
RE.CNT 16   THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
             ALL CITATIONS AVAILABLE IN THE RE FORMAT

> d ab

L16 ANSWER 1 OF 1 CA COPYRIGHT 2004 ACS on STN
AB Major, minor, and trace elements in 60 native Au samples from across
    Canada were analyzed directly by laser ablation microprobe inductively
    coupled plasma-mass spectrometry (LAM-ICP-MS). Diams. of laser ablation
    craters ranged from 100 to 150 μm defining the smallest sample size
    determinable. The Au signal was used as an internal standard to correct for
    differences in ablation yields, matrix effects and signal **drift**
    during anal. Anal. results obtained over a period of seven months for the
    synthetic Au alloy standard 501 demonstrated the long-term reproducibility of
    the method. The elemental signatures obtained from individual
    specimens have proven to be unique and reproducible, yielding data
    that can be used for matching "unknowns" with their source location.

> d 14 4

L4   ANSWER 4 OF 4 CA COPYRIGHT 2004 ACS on STN
N   124:81135 CA
I   Correction of Mass Spectral **Drift** Using Artificial Neural
    Networks
U   **Goodacre, Royston**; Kell, Douglas B.
S   Institute of Biological Sciences, University of Wales, Aberystwyth/Dyfed,
    SY23 3DA, UK
O   Analytical Chemistry (1996), 68(2), 271-80
    CODEN: ANCHAM; ISSN: 0003-2700
PB American Chemical Society
T   Journal
A   English

> log y
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                      ENTRY   SESSION

ULL ESTIMATED COST   122.93   124.28

ISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)   SINCE FILE   TOTAL
                                                      ENTRY   SESSION
A SUBSCRIBER PRICE   -7.92   -7.92

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                     resulting in a closer connection to BABS
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                     fields
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                     Patent Office Classifications
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 NEWS   9   SEP 01 INPADOC: New family current-awareness alert (SDI) available
 NEWS 10   SEP 01 New pricing for the Save Answers for SciFinder Wizard within
                     STN Express with Discover!
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 NEWS 12   SEP 27 STANDARDS will no longer be available on STN
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 NEWS 14   OCT 28 KOREAPAT now available on STN

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                MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
                AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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 NEWS INTER   General Internet Information
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 NEWS WWW   CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 14:52:08 ON 15 NOV 2004

=> file medline
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                       ENTRY   SESSION
FULL ESTIMATED COST   0.21   0.21

FILE 'MEDLINE' ENTERED AT 14:52:40 ON 15 NOV 2004

 FILE LAST UPDATED: 13 NOV 2004 (20041113/UP). FILE COVERS 1950 TO DATE.

 On February 29, 2004, the 2004 MeSH terms were loaded. See HELP RLOAD

for details.

OLDMEDLINE now back to 1950.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the
MeSH 2004 vocabulary. See http://www.nlm.nih.gov/mesh/ and
http://www.nlm.nih.gov/pubs/techbull/nd03/nd03_mesh.html for a
description of changes.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

```
=> e goodacre/au
E1              1     GOODA K/AU
E2              2     GOODA S A/AU
E3              0 --> GOODACRE/AU
E4             22     GOODACRE A/AU
E5              6     GOODACRE A M/AU
E6              1     GOODACRE ANGELA/AU
E7             10     GOODACRE B/AU
E8              2     GOODACRE B B/AU
E9              1     GOODACRE B C/AU
E10            20     GOODACRE B W/AU
E11             1     GOODACRE BRIAN/AU
E12             4     GOODACRE BRIAN W/AU

=> e goodacre royston/au
E1              4     GOODACRE R H/AU
E2             17     GOODACRE R L/AU
E3             22 --> GOODACRE ROYSTON/AU
E4             24     GOODACRE S/AU
E5              1     GOODACRE S C/AU
E6              2     GOODACRE S H/AU
E7              2     GOODACRE S L/AU
E8             11     GOODACRE S W/AU
E9              1     GOODACRE SARA L/AU
E10             7     GOODACRE STEVE/AU
E11             1     GOODACRE STEVE W/AU
E12            14     GOODACRE T/AU

=> s e3
L1             22 "GOODACRE ROYSTON"/AU

=> d ti 1-22
```

L1   ANSWER 1 OF 22   MEDLINE on STN
TI   Differentiation of Micromonospora Isolates from a Coastal Sediment in
      Wales on the Basis of Fourier Transform Infrared Spectroscopy, 16S rRNA
      Sequence Analysis, and the Amplified Fragment Length Polymorphism
      Technique.

L1   ANSWER 2 OF 22   MEDLINE on STN
TI   Comparison of diffuse-reflectance absorbance and attenuated total
      reflectance FT-IR for the discrimination of bacteria.

L1   ANSWER 3 OF 22   MEDLINE on STN
TI   Surface-enhanced Raman spectroscopy for bacterial discrimination utilizing
      a scanning electron microscope with a Raman spectroscopy interface.

L1   ANSWER 4 OF 22   MEDLINE on STN
TI   Selective detection of proteins in mixtures using electrospray ionization
      mass spectrometry: influence of instrumental settings and implications for
      proteomics.

L1   ANSWER 5 OF 22   MEDLINE on STN
TI   Metabolomics by numbers: acquiring and understanding global metabolite
      data.

L1   ANSWER 6 OF 22   MEDLINE on STN

I Whole-organism fingerprinting of the genus Carnobacterium using Fourier
 transform infrared spectroscopy (FT-IR).

1 ANSWER 7 OF 22 MEDLINE on STN
I Ultra-violet resonance Raman spectroscopy for the rapid discrimination of
 urinary tract infection bacteria.

1 ANSWER 8 OF 22 MEDLINE on STN
I Metabolic profiling: pathways in discovery.

1 ANSWER 9 OF 22 MEDLINE on STN
I Characterization of microorganisms using UV resonance Raman spectroscopy
 and chemometrics.

1 ANSWER 10 OF 22 MEDLINE on STN
I Discrimination of bacteria using surface-enhanced Raman spectroscopy.

1 ANSWER 11 OF 22 MEDLINE on STN
I Application of high-throughput Fourier-transform infrared spectroscopy in
 toxicology studies: contribution to a study on the development of an
 animal model for idiosyncratic toxicity.

1 ANSWER 12 OF 22 MEDLINE on STN
I Explanatory optimization of protein mass spectrometry via genetic search.

1 ANSWER 13 OF 22 MEDLINE on STN
I Rapid quantitative assessment of the adulteration of virgin olive oils
 with hazelnut oils using Raman spectroscopy and chemometrics.

1 ANSWER 14 OF 22 MEDLINE on STN
I Investigating plant-plant interference by metabolic fingerprinting.

1 ANSWER 15 OF 22 MEDLINE on STN
I Metabolic fingerprinting of salt-stressed tomatoes.

1 ANSWER 16 OF 22 MEDLINE on STN
I Chemometric discrimination of unfractionated plant extracts analyzed by
 electrospray mass spectrometry.

1 ANSWER 17 OF 22 MEDLINE on STN
I Metabolic profiling using direct infusion electrospray ionisation mass
 spectrometry for the characterisation of olive oils.

1 ANSWER 18 OF 22 MEDLINE on STN
I Fluorescent amplified fragment length polymorphism probabilistic database
 for identification of bacterial isolates from urinary tract infections.

1 ANSWER 19 OF 22 MEDLINE on STN
I Monitoring of complex industrial bioprocesses for metabolite
 concentrations using modern spectroscopies and machine learning:
 application to gibberellic acid production.

1 ANSWER 20 OF 22 MEDLINE on STN
I Sample preparation in matrix-assisted laser desorption/ionization mass
 spectrometry of whole bacterial cells and the detection of high mass (>20
 kDa) proteins.

1 ANSWER 21 OF 22 MEDLINE on STN
I Rapid and quantitative detection of the microbial spoilage of meat by
 fourier transform infrared spectroscopy and machine learning.

1 ANSWER 22 OF 22 MEDLINE on STN
I Flow-injection electrospray ionization mass spectrometry of crude cell
 extracts for high-throughput bacterial identification.

> s l1 and drift
   5370 DRIFT
2   0 L1 AND DRIFT

> e goodacre r/au
```
1           7     GOODACRE JOHN A/AU
2           1     GOODACRE PAUL R/AU
3          19 --> GOODACRE R/AU
4           1     GOODACRE ROBERT/AU
5           1     GOODACRE ROBERT L/AU
6          86     GOODACRE ROYSTON/AU
7           1     GOODACRE S/AU
8          .1     GOODACRE SARA/AU
9           1     GOODACRE SARA L/AU
10          2     GOODACRE SIMON/AU
11          3     GOODACRE SIMON C/AU
12         21     GOODACRE SIMON CHARLES/AU
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> s e6
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3          86 "GOODACRE ROYSTON"/AU
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> s drift and l3
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       34318 DRIFT
4           4 DRIFT AND L3
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> d ti 1-4

4   ANSWER 1 OF 4   CA   COPYRIGHT 2004 ACS on STN
I   On mass spectrometer instrument standardization and interlaboratory
     calibration transfer using neural networks

4   ANSWER 2 OF 4   CA   COPYRIGHT 2004 ACS on STN
I   Rapid analysis of multiple determinands using pyrolysis mass spectrometry
     and supervised learning with artificial neural networks - principles and
     applications

4   ANSWER 3 OF 4   CA   COPYRIGHT 2004 ACS on STN
I   Analyzing a sample by using a neural network to correct for measurement
     drift

4   ANSWER 4 OF 4   CA   COPYRIGHT 2004 ACS on STN
I   Correction of Mass Spectral **Drift** Using Artificial Neural
     Networks

ANSWER 1 OF 4   CA   COPYRIGHT 2004 ACS on STN
For pyrolysis mass spectrometry (PyMS) to be exploited in areas such as
the routine identification of microorganisms, for quantifying determinants
in biol. and biotechnol. systems, and in the production of useful mass
spectral libraries, it is paramount that newly acquired spectra be
comparable to those previously collected and held in a central reference laboratory
Artificial neural networks (ANNs) and other multivariate calibration
models have been used to relate mass spectra to the biol. features of
interest.   However, calibration models developed on one mass spectrometer
cannot be used with spectra collected on a second instrument, because of
the differences between the instrumental responses of both instruments.
We report here that an ANN-based **drift** correction procedure can
be implemented so that newly acquired spectra can be used to challenge
models constructed using mass spectra collected on different instruments.
Calibration samples were run on three different PyMS machines, and ANNs
set up in which the inputs were the 150 machine 'a' calibration masses and
the outputs were the 150 calibration masses from the machine 'b' spectra.
Such associative neural networks could thus be used as signal-processing
elements to effect the transformation of data acquired on one machine to
those which would have been acquired on a different instrument.
Therefore, for the first time PyMS could be used to acquire spectra which
could usefully be compared to those previously collected and held in a
data-base, irresp. of the mass spectrometer used.   The examples reported
are for the quant. assessment of the amount of lysozyme in a binary mixture
with glycogen and the rapid identification down to the species level of
bacteria belonging to the genus Eubacterium.   This approach is not limited
solely to pyrolysis mass spectrometry but is generally applicable to any
anal. tool which is prone to deterioration in calibration transfer, such
as IR, ESR, NMR and other vibrational spectroscopies, gas and liquid
chromatog., as well as other types of mass spectrometry.

ANSWER 2 OF 4   CA   COPYRIGHT 2004 ACS on STN
Curie-point pyrolysis mass spectrometry is a rapid, high-resolution technique
which has enjoyed historical success in the operational fingerprinting and
classification of microbial and other biol. systems.   More recently we
have exploited the anal. power of this technique together with supervised
learning, based on artificial neural networks and cognate chemometric
methods, for the accurate and quant. anal. of complex biol. materials,
including microorganisms, fermentor broths and agricultural products.
When suitable stds. are available, supervised learning is much more
powerful than in unsupervised learning for the chemometric anal. of
multivariate spectroscopic data.   Similar neural network methods may also
be used to correct for mass spectral **drift.**

ANSWER 3 OF 4   CA   COPYRIGHT 2004 ACS on STN
A method and apparatus are disclosed for analyzing a sample in which a neural
network is trained to correct for measurement **drift** of a given
anal. instrument (e.g., a mass spectrometer).   The training is done by
using first and second sets of data obtained by the instrument from
samples of known compns. at initial and subsequent instants of time, resp.
The trained network is used to transform data, obtained by the instrument
from a sample of unknown composition at said subsequent instant of time, to an
estimate of the data which would have been obtained by the instrument from
that sample at the initial instant of time.   The transformed data then are
analyzed to analyze the sample of unknown composition   Examples are given of
the use of pyrolysis mass spectrometry for the determination of lysozyme and
glycogen in mixture, ampicillin in Escherichia coli, Staphylococcus aureus
in mixts. with Escherichia coli, and identification of human isolates of
Propionibacterium acnes.

ANSWER 4 OF 4   CA   COPYRIGHT 2004 ACS on STN
For pyrolysis mass spectrometry (PyMS) to be used for the routine
identification of microorganisms, for quantifying determinands in biol.
and biotechnol. systems, and in the production of useful mass spectral
libraries, it is paramount that newly acquired spectra be compared to
those previously collected.   Neural network and other multivariate

calibration models have been used to relate mass spectra to the biol.
features of interest. As commonly observed, however, mass spectral
fingerprints showed a lack of long-term reproducibility due to
instrumental **drift** in the mass spectrometer; when identical
materials were analyzed by PyMS at dates from 4 to 20 mo apart, neural
network models produced at earlier times could not be used to give
accurate ests. of determinand concns. or bacterial identities. Neural
networks, however, can be used to correct for pyrolysis mass spectrometer
instrumental **drift** itself, so that neural network or other
multivariate calibration models created using previously collected data
can be used to give accurate ests. of determinand concentration or the nature of
bacteria (or, indeed, other materials) from newly acquired pyrolysis mass
spectra. This approach is not limited solely to pyrolysis mass
spectrometry but is generally applicable to any anal. tool which is prone
to instrumental **drift**, such as IR, ESR, NMR and other
spectroscopies, and gas and liquid chromatog., as well as other types of
mass spectrometry.

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=>
=> e wilkes j/au
E1            2     WILKES IAN PETER/AU
E2            1     WILKES INGO/AU
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E4            4     WILKES J B/AU
E5            3     WILKES J D/AU
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=> e
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E16           1     WILKES JAMES E/AU
E17           4     WILKES JAMES M/AU
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E23           1     WILKES JENNIFER J/AU
E24           3     WILKES JILLIAN/AU

=> e
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E36           1     WILKES JOHN STEPHEN/AU

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E39           2     WILKES JON/AU
E40          27     WILKES JON G/AU
E41           1     WILKES JON GARDNER/AU
E42           1     WILKES JONATHAN/AU
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45        2      WILKES K/AU
46        6      WILKES K E/AU
47        1      WILKES K TREVOR/AU
48        1      WILKES KARL A/AU

> s e39-e41
          2   "WILKES JON"/AU
         27   "WILKES JON G"/AU
          1   "WILKES JON GARDNER"/AU
.5       30   ("WILKES JON"/AU OR "WILKES JON G"/AU OR "WILKES JON GARDNER"/AU
              )

> d ti 1-30

.5    ANSWER 1 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    Predicting toxic equivalence factors from 13C nuclear magnetic resonance
      spectra for dioxins, furans, and polychlorinated biphenyls using linear
      and nonlinear pattern recognition methods

.5    ANSWER 2 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    Using Simulated 2D 13C NMR Nearest Neighbor Connectivity Spectral Data
      Patterns to Model a Diverse Set of Estrogens

.5    ANSWER 3 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    Carbon-13 COSY NMR data for quantitative structure-activity relationships
      and quantitative molecular structure-property relationships of
      biomolecules

.5    ANSWER 4 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    Combining NMR spectral and structural data to form models of
      polychlorinated dibenzodioxins, dibenzofurans, and biphenyls binding to
      the AhR

.5    ANSWER 5 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    The use of carbon thirteen nuclear magnetic resonance spectra to predict
      dioxin and furan binding affinities to the aryl hydrocarbon receptor

.5    ANSWER 6 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    Chemistry in aldol complexes of metal dications: dehydration of the
      bisligand species

.5    ANSWER 7 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    Comparative structural connectivity spectra analysis (CoSCoSA) models of
      steroids binding to the aromatase enzyme

.5    ANSWER 8 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    Defining and using microbial spectral databases

.5    ANSWER 9 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    Microbial identification databases

.5    ANSWER 10 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    Comparative structural connectivity spectra analysis (CoSCoSA) models of
      steroid binding to the corticosteroid binding globulin

.5    ANSWER 11 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    Fragmentation Chemistry of DMSO Complexes of Metal Dications

.5    ANSWER 12 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    Fragmentation and charge transfer in gas-phase complexes of divalent metal
      ions with acetonitrile

.5    ANSWER 13 OF 30   CA   COPYRIGHT 2004 ACS on STN
'I    Prediction of toxic equivalency factors for dioxins, furans and PCBs using
      artificial neural networks

.5    ANSWER 14 OF 30   CA   COPYRIGHT 2004 ACS on STN
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TI   Developing 13C NMR quantitative spectrometric data-activity relationship
      (QSDAR) models of steroid binding to the corticosteroid binding globulin

L5   ANSWER 15 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   13C NMR Quantitative Spectrometric Data-Activity Relationship (QSDAR)
 .   Models of Steroids Binding the Aromatase Enzyme

L5   ANSWER 16 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Models of Polychlorinated Dibenzodioxins, Dibenzofurans, and Biphenyls
      Binding Affinity to the Aryl Hydrocarbon Receptor Developed Using 13C NMR
      Data

L5   ANSWER 17 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   13C NMR and Electron Ionization Mass Spectrometric Data-Activity
      Relationship Model of Estrogen Receptor Binding

L5   ANSWER 18 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Use of 13C NMR Spectrometric Data To Produce a Predictive Model of
      Estrogen Receptor Binding Activity

L5   ANSWER 19 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Electrospray mass spectrometry for mycotoxin detection and purity analysis

L5   ANSWER 20 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Producing 13C NMR, Infrared Absorption, and Electron Ionization Mass
      Spectrometric Data Models of the Monodechlorination of Chlorobenzenes,
      Chlorophenols, and Chloroanilines

L5   ANSWER 21 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Food quality indicator device to detect volatile amines

L5   ANSWER 22 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Sample preparation and high-resolution separation of mycotoxins possessing
      carboxyl groups

L5   ANSWER 23 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Long-term occurrence of Trypanosoma congolense resistance to diminazene,
      isometamidium and homidium in cattle at Ghibe, Ethiopia

L5   ANSWER 24 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Determination of underivatized fumonisin B1 and related compounds by HPLC

L5   ANSWER 25 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Multiresidue analysis of pesticides by electrospray LC-MS and LC-MS-MS

L5   ANSWER 26 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Diffusion based solvent removal interface for coupling liquid and
      supercritical fluid chromatography to gas chromatographic detectors

L5   ANSWER 27 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   AC corona-discharge aerosol-neutralization device adapted to liquid
      chromatography/particle beam/mass spectrometry

L5   ANSWER 28 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Particle size distribution is not the major factor explaining variable
      analyte transmission efficiency in liquid chromatography/particle
      beam/mass spectrometry

L5   ANSWER 29 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Determination of fumonisins B1, B2, B3 and B4 by high-performance liquid
      chromatography with evaporative light-scattering detection

L5   ANSWER 30 OF 30   CA   COPYRIGHT 2004 ACS on STN
TI   Application of the particle beam interface to high-performance liquid
      chromatography-thermal energy analysis and electron impact mass
      spectrometry for detection of non-volatile N-nitrosamines

=> s drift and 15

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       34318 DRIFT
L6        1 DRIFT AND L5

=> d


L6    ANSWER 1 OF 1   CA   COPYRIGHT 2004 ACS on STN
AN    137:228971  CA
TI    Microbial identification databases
IN    Wilkes, Jon G.; Rafii, Fatemeh; Glover, Katherine L.; Holcomb,
      Manuel; Cao, Xiaoxi; Sutherland, John B.
PA    The Government of the United States of America, USA
SO    U.S. Pat. Appl. Publ., 41 pp.
      CODEN: USXXCO
DT    Patent
LA    English
FAN.CNT 1
      PATENT NO.          KIND    DATE      APPLICATION NO.        DATE
      ---------------     ----    --------  --------------------   --------
PI    US 2002138210       A1      20020926  US 2001-975530         20011010
PRAI  US 2000-239549P     P       20001010


=> s identification and drift
        273269 IDENTIFICATION
         34318 DRIFT
L7         528 IDENTIFICATION AND DRIFT

=> d ti 1-10

L7    ANSWER 1 OF 528   CA   COPYRIGHT 2004 ACS on STN
TI    Implications of molecular genotyping of Helicobacter pylori isolates from
      different human populations by genomic fingerprinting of enterobacterial
      repetitive intergenic consensus regions for strain identification
      and geographic evolution

L7    ANSWER 2 OF 528   CA   COPYRIGHT 2004 ACS on STN
TI    Apparatus and method for focusing and selecting ions and charged particles
      at or near atmospheric pressure

L7    ANSWER 3 OF 528   CA   COPYRIGHT 2004 ACS on STN
TI    Development of a Plutonium Ceramic Target for the MASHA Separator

L7    ANSWER 4 OF 528   CA   COPYRIGHT 2004 ACS on STN
TI    Electrospray Ionization Ion Mobility Spectrometry of Amino Acids: Ion
      Mobilities and a Mass-Mobility Correlation

L7    ANSWER 5 OF 528   CA   COPYRIGHT 2004 ACS on STN
TI    $\Lambda$ production at high rapidity in d + Au collisions at $\sqrt{s_{NN}}$ =
      200 GeV

L7    ANSWER 6 OF 528   CA   COPYRIGHT 2004 ACS on STN
TI    Improved identification of conjugated linoleic acid isomers
      using silver-ion HPLC separations

L7    ANSWER 7 OF 528   CA   COPYRIGHT 2004 ACS on STN
TI    Basic instrumentation for Hall A at Jefferson Lab

L7    ANSWER 8 OF 528   CA   COPYRIGHT 2004 ACS on STN
TI    Temperature-modulated gas sensors: selection of modulating frequencies
      through noise methods

L7    ANSWER 9 OF 528   CA   COPYRIGHT 2004 ACS on STN
TI    Status of design and construction of the Transition Radiation Tracker
      (TRT) for the ATLAS experiment at the LHC

L7    ANSWER 10 OF 528   CA   COPYRIGHT 2004 ACS on STN
TI    A straw drift chamber spectrometer for studies of rare kaon
      decays
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=> s sample drift
SAMPLE IS IGNORED AS A SCOPE FOR THIS SEARCH
L8          34318 DRIFT

=> d 17 ab

L7    ANSWER 1 OF 528  CA  COPYRIGHT 2004 ACS on STN
AB    Biogeog. partitioning of the genome is typical of the gastric pathogen
      Helicobacter pylori.  Such population-specific evolution could serve as a
      model for understanding host-pathogen interaction and the impact of
      genetic drift and recombination on insular populations.  With a
      total of 320 isolates from six geog. regions (Japan, India, England,
      Spain, Ireland, Africa, and Peru) analyzed by enterobacterial repetitive
      intergenic consensus (ERIC)-based genotyping, we examined genetic affinities
      among various H. pylori populations in the world.  Several strain-specific
      and region-specific differences were observed by ERIC-based typing.
      Polymorphic ERIC patterns indicated that the ERIC sequences are in fact
      dispersed in the H. pylori chromosome at different locations separated by
      various distances.  Phylogenetic anal. of 61 representative isolates
      revealed three distinct genetic clusters populated by isolates with shared
      ERIC types independent of the cag right-junction motif type and vacA
      allele status.  Among the notable genetic relationships were the genotypic
      similarities between Irish and Japanese and between Peruvian and Japanese
      isolates.  Insular genotypic characteristics of Irish isolates amid
      genetic similarity to East Asian, as well as North European, strains have
      been once again proved in this study.  Peruvian genotypes were more
      similar to those of Japanese isolates than to those of Iberian or European
      isolates.  Given the current debate on the origin and age of present-day
      H. pylori, this is a significant finding that supports the possibility of
      ancient colonization of Amerindians with East Asian strains.  Genotypic
      data presented here will be addnl. helpful in realizing the importance of
      H. pylori geog. genomics in the development of gastro-duodenal pathol.


=> s mass spect? and 18
          799626 MASS
         2316030 SPECT?
          260887 MASS SPECT?
                 (MASS(W)SPECT?)
L9           1126 MASS SPECT? AND L8

=> d ti 1-10

L9    ANSWER 1 OF 1126  CA  COPYRIGHT 2004 ACS on STN
TI    Resolution equations for high-field ion mobility

L9    ANSWER 2 OF 1126  CA  COPYRIGHT 2004 ACS on STN
TI    Nanoflow LC/IMS-MS and LC/IMS-CID/MS of protein mixtures

L9    ANSWER 3 OF 1126  CA  COPYRIGHT 2004 ACS on STN
TI    Development of Ion Drift-Chemical Ionization Mass
      Spectrometry

L9    ANSWER 4 OF 1126  CA  COPYRIGHT 2004 ACS on STN
TI    Construction and evaluation of polar-angle-resolved miniature
      time-of-flight ion mass spectrometer, and its
      application for electron-ion coincidence spectroscopy

L9    ANSWER 5 OF 1126  CA  COPYRIGHT 2004 ACS on STN
TI    Electron attachment to and anion reactions with SF5Cl: electron-swarm and
      selected ion flow tube studies

L9    ANSWER 6 OF 1126  CA  COPYRIGHT 2004 ACS on STN
TI    Peak capacity of ion mobility mass spectrometry: the
      utility of varying drift gas polarizability for the separation
      of tryptic peptides

L9    ANSWER 7 OF 1126  CA  COPYRIGHT 2004 ACS on STN
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TI   Soybean foliage residues of dicamba and 2,4-D and correlation to
      application rates and yield

L9   ANSWER 8 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   In situ **mass spectrometry** in a 10 Torr W chemical
      vapor deposition process for film thickness metrology and real-time
      advanced process control

L9   ANSWER 9 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   **Mass spectrometers**

L9   ANSWER 10 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   Efficient direct current collision and reaction cell

=> d ti 11-20

L9   ANSWER 11 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   Apparatus and method for focusing and selecting ions and charged particles
      at or near atmospheric pressure

L9   ANSWER 12 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   Determination of thorium and uranium in Chinese foods by inductively
      coupled plasma **mass spectrometry**

L9   ANSWER 13 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   Method and apparatus for efficient transfer of ions into a **mass
      spectrometer**

L9   ANSWER 14 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   Time-of-flight **mass spectrometer**

L9   ANSWER 15 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   Electrospray Ionization Ion Mobility Spectrometry of Amino Acids: Ion
      Mobilities and a Mass-Mobility Correlation

L9   ANSWER 16 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   Multidynamic isotope ratio analysis using MC-ICP-MS and the causes of
      secular **drift** in Hf, Nd and Pb isotope ratios

L9   ANSWER 17 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   CeO2 catalysed soot oxidation. The role of active oxygen to accelerate the
      oxidation conversion

L9   ANSWER 18 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   Dissociation pathways of protonated water clusters

L9   ANSWER 19 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   Demonstration of Proton-Transfer Reaction Time-of-Flight **Mass
      Spectrometry** for Real-Time Analysis of Trace Volatile Organic
      Compounds

L9   ANSWER 20 OF 1126   CA   COPYRIGHT 2004 ACS on STN
TI   Compositional analysis of isobutylene/p-methylstyrene copolymers by
      matrix-assisted laser desorption/ionization **mass
      spectrometry**

=> s fingerprint and 19
          6620 FINGERPRINT
L10   2 FINGERPRINT AND L9

=> d ti 1-2

L10   ANSWER 1 OF 2   CA   COPYRIGHT 2004 ACS on STN
TI   Microbial identification databases
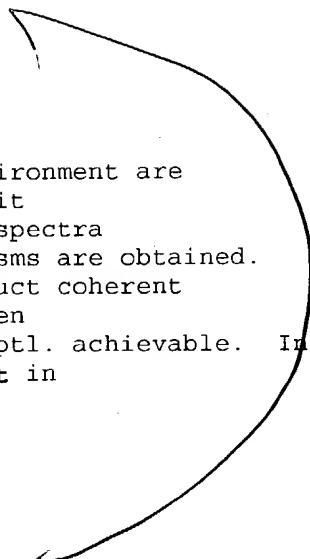
L10   ANSWER 2 OF 2   CA   COPYRIGHT 2004 ACS on STN
TI   Gas Sensors Arrays ('Electronic Noses'): a study about the speed/accuracy

```
        ratio

=> d 1 ab

L10  ANSWER 1 OF 2   CA   COPYRIGHT 2004 ACS on STN
AB   Methods of compensating for **drift** in **fingerprint**
     spectra of microorganisms caused by changes in their environment are
     disclosed.  These methods of compensating for **drift** permit
     identification of microorganisms from their **fingerprint** spectra
     regardless of the environment from which the microorganisms are obtained.
     Furthermore, the disclosed methods may be used to construct coherent
     databases of **fingerprint** spectra that may be expanded even
     though the standard database conditions are no longer exptl. achievable.  In
     particular embodiments, methods of compensating for **drift** in
     pyrolysis **mass spectra**, constructing coherent
     pyrolysis **mass spectral** databases, and identifying
     bacteria from their pyrolysis **mass spectra** are
     disclosed.


=> d

L10   ANSWER 1 OF 2   CA   COPYRIGHT 2004 ACS on STN
AN    137:228971   CA
TI    Microbial identification databases
IN    Wilkes, Jon G.; Rafii, Fatemeh; Glover, Katherine L.; Holcomb, Manuel;
      Cao, Xiaoxi; Sutherland, John B.
PA    The Government of the United States of America, USA
SO    U.S. Pat. Appl. Publ., 41 pp.
      CODEN: USXXCO
DT    Patent
LA    English
FAN.CNT 1
      PATENT NO.            KIND    DATE      APPLICATION NO.        DATE
      ---------------       ----    --------  --------------------   --------
PI    US 2002138210         A1      20020926  US 2001-975530         20011010
PRAI  US 2000-239549P       P       20001010


=> s specimen
L11       91655 SPECIMEN

=> d his

      (FILE 'HOME' ENTERED AT 14:52:08 ON 15 NOV 2004)

      FILE 'MEDLINE' ENTERED AT 14:52:40 ON 15 NOV 2004
                E GOODACRE/AU
                E GOODACRE ROYSTON/AU
L1         22 S E3
L2          0 S L1 AND DRIFT

      FILE 'CA' ENTERED AT 14:54:30 ON 15 NOV 2004
                E GOODACRE R/AU
L3         86 S E6
L4          4 S DRIFT AND L3
                E WILKES J/AU
L5         30 S E39-E41
L6          1 S DRIFT AND L5
L7        528 S IDENTIFICATION AND DRIFT
L8      34318 S SAMPLE DRIFT
L9       1126 S MASS SPECT? AND L8
L10         2 S FINGERPRINT AND L9
L11     91655 S SPECIMEN

=> s l11 and l8
L12       213 L11 AND L8
```

L2   ANSWER 1 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   Development of coincidence transmission electron microscope. III.
     Incorporation with γ-type imaging energy filter

L2   ANSWER 2 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   Improvesments in dimensional stability and lightfastness of wood by
     butyrylation using microwave heating

L2   ANSWER 3 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   Analytical electron microscopy of InP/(In, Ga)As heterogeneous structures

L2   ANSWER 4 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   The use of environmental scanning electron microscopy for imaging wet and
     insulating materials

L2   ANSWER 5 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   Investigation of the change in the **DRIFT** spectra of
     light-irradiated wood with heat treatment

L2   ANSWER 6 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   Characteristics of carrier mobility in polyaniline

L2   ANSWER 7 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   Surface Modification of Colloidal Silica by Sulfonation Route for
     Super-Hydrophilicity

L2   ANSWER 8 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   Characterization of metal-ceramic interfaces using low voltage x-ray
     microanalysis in a field emission scanning electron microscope

L2   ANSWER 9 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   **Drift** in the hypervariable region of the hepatitis C virus
     during 27 years in two patients

L2   ANSWER 10 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   Electron **drift** mobility in polystyrene doped with
     bispyrazolopyridine derivatives

L2   ANSWER 11 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   A new method for the determination of the wave aberration function for
     high resolution TEM 1. Measurement of the symmetric aberrations

L2   ANSWER 12 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   A **specimen-drift**-free EDX mapping system in a STEM for
     observing two-dimensional profiles of low dose elements in fine
     semiconductor devices

L2   ANSWER 13 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   Automated Data Collection with a Tecnai 12 Electron Microscope:
     Applications for Molecular Imaging by Cryomicroscopy

L2   ANSWER 14 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   Automated analysis of submicron particles by CCSEM / EDXS - where are the
     limits?

L2   ANSWER 15 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   Automated analysis of submicron particles by computer-controlled scanning
     electron microscopy

L2   ANSWER 16 OF 213   CA   COPYRIGHT 2004 ACS on STN
I   Scanning probe microscope, method for measuring band structure of
     substance by using the microscope, and microscopic spectroscopy

L2   ANSWER 17 OF 213   CA   COPYRIGHT 2004 ACS on STN

TI   Step bunching, step wandering and faceting. Self-organization at Si
     surfaces

L2   ANSWER 18 OF 213   CA   COPYRIGHT 2004 ACS on STN
TI   Analysis of nanoscale multilayers by EDXS and EELS in the STEM

L2   ANSWER 19 OF 213   CA   COPYRIGHT 2004 ACS on STN
TI   The adsorption and curing behaviors of the epoxy/amidoamine system in the
     presence of metal oxides

L2   ANSWER 20 OF 213   CA   COPYRIGHT 2004 ACS on STN
TI   A novel multicell silicon **drift** detector module for x-ray
     spectroscopy and imaging applications

=> d ab 12

L2   ANSWER 12 OF 213   CA   COPYRIGHT 2004 ACS on STN
AB   We developed a **specimen-drift**-free energy-dispersive
     X-ray (EDX) mapping system in a scanning transmission electron microscope
     (STEM) to improve the sensitivity and spatial resolution of EDX elemental
     mapping images. The amount of **specimen drift** was
     analyzed from two STEM images before and after **specimen**
     drift by using the phase-correlation method, and was compensated
     for with an image-shift deflector of the STEM by the displacement of the
     scanning electron beam. We applied this system to observe the
     two-dimensional distribution of low dose arsenic in silicon semiconductor
     devices. The sensitivity of the elemental mapping was improved to several
     tenths atomic % for arsenic atoms while maintaining a spatial resolution of 2
     nm.

=> d l12 and fingerprint?
'AND' IS NOT A VALID FORMAT FOR FILE 'CA'
'FINGERPRINT?' IS NOT A VALID FORMAT FOR FILE 'CA'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
AN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, IPC, and NCL

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

BIB --------- BIB, no citations
IBIB -------- IBIB, no citations

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IT --------- Fields containing hit terms
ITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
ITRN ------- HIT RN and its text modification
ITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
ITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
HITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
WIC -------- Hit term plus 20 words on either side
CC --------- Number of occurrence of hit term and field in which it occurs

o display a particular field or fields, enter the display field
odes.  For a list of the display field codes, enter HELP DFIELDS at
n arrow prompt (=>).  Examples of formats include: TI; TI,AU; BIB,ST;
I,IND; TI,SO.  You may specify the format fields in any order and the
nformation will be displayed in the same order as the format
pecification.

ll of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR,
HITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC
o view a specified Accession Number.
NTER DISPLAY FORMAT (BIB):
NTER DISPLAY FORMAT (BIB):bib

12   ANSWER 1 OF 213  CA   COPYRIGHT 2004 ACS on STN
N    141:342470  CA
I    Development of coincidence transmission electron microscope. III.
     Incorporation with γ-type imaging energy filter
U    Nishinaka, Kenichi; Taka, Shinsuke; Kimura, Yoshihide; Takai, Yoshizo
S    Department of Material and Life Science, Graduate School of Engineering,
     Osaka University, Suita, Osaka, 565-0871, Japan
O    Journal of Electron Microscopy (2004), 53(3), 217-222
     CODEN: JELJA7; ISSN: 0022-0744
B    Oxford University Press
T    Journal
A    English
E.CNT  11     THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT


> s 112 and fingerprint?
         16668 FINGERPRINT?
13           0 L12 AND FINGERPRINT?

> d his

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     FILE 'MEDLINE' ENTERED AT 14:52:40 ON 15 NOV 2004
               E GOODACRE/AU
               E GOODACRE ROYSTON/AU
1         22 S E3
2          0 S L1 AND DRIFT

     FILE 'CA' ENTERED AT 14:54:30 ON 15 NOV 2004
               E GOODACRE R/AU
3         86 S E6
4          4 S DRIFT AND L3
               E WILKES J/AU
5         30 S E39-E41
6          1 S DRIFT AND L5
7        528 S IDENTIFICATION AND DRIFT
8      34318 S SAMPLE DRIFT
9       1126 S MASS SPECT? AND L8
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       2 S FINGERPRINT AND L9
   91655 S SPECIMEN
     213 S L11 AND L8
       0 S L12 AND FINGERPRINT?
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sted terms that are not separated by a logical operator.

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   34318 DRIFT
   16668 FINGERPRINT?
       0 DRIFT AND FINGERPRINT? AND L11
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s drift and fingerprint?
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   34318 DRIFT
   16668 FINGERPRINT?
      41 DRIFT AND FINGERPRINT?
```

d ti 1-10

ANSWER 1 OF 41   CA   COPYRIGHT 2004 ACS on STN
Implications of molecular genotyping of Helicobacter pylori isolates from
different human populations by genomic **fingerprinting** of
enterobacterial repetitive intergenic consensus regions for strain
identification and geographic evolution

ANSWER 2 OF 41   CA   COPYRIGHT 2004 ACS on STN
Silylation and surface properties of chemically grafted hydrophobic silica

ANSWER 3 OF 41   CA   COPYRIGHT 2004 ACS on STN
Population genetic structure of Titanotrichum oldhamii (Gesneriaceae), a
subtropical bulbiliferous plant with mixed sexual and asexual reproduction

ANSWER 4 OF 41   CA   COPYRIGHT 2004 ACS on STN
Molecular epidemiology and diagnosis of Leishmania: what have we learnt
from genome structure, dynamics and function?

ANSWER 5 OF 41   CA   COPYRIGHT 2004 ACS on STN
Genetic diversity of selected bacterial populations in North Carolina

ANSWER 6 OF 41   CA   COPYRIGHT 2004 ACS on STN
Microbial identification databases

ANSWER 7 OF 41   CA   COPYRIGHT 2004 ACS on STN
Nonlinear electrophoresis and focusing of macromolecules

ANSWER 8 OF 41   CA   COPYRIGHT 2004 ACS on STN
Interpretation of band differences to distinguish strains of Serratia
marcescens by pulsed-field gel electrophoresis of XbaI DNA digests

ANSWER 9 OF 41   CA   COPYRIGHT 2004 ACS on STN
Gas Sensors Arrays ('Electronic Noses'): a study about the speed/accuracy
ratio

ANSWER 10 OF 41   CA   COPYRIGHT 2004 ACS on STN
Low RAPD polymorphism in Archangiopteris itoi, a rare and endemic fern in
Taiwan

d ab 8

ANSWER 8 OF 41   CA   COPYRIGHT 2004 ACS on STN
The number of band differences in DNA macrorestriction profiles required to
distinguish unrelated strains from an index strain varies in an outbreak
with the species and restriction enzyme used. In order to define this
difference for epidemiol. studies of Serratia marcescens, we produced DNA
fingerprints from 57 isolates of the organism using the

restriction enzyme XbaI and pulsed-field gel electrophoresis (PFGE). The
isolates were selected on the basis of their epidemiol., serotype and
phage-typing patterns to include 28 unrelated strains and 29
representatives from 2 distinct outbreaks. One of the outbreaks was
prolonged, lasting for several years. Electrophoretic profiles consisting
of 20 or more clearly resolved bands were obtained for all isolates.
Twenty-six of the unrelated strains had unique profiles with over 10 band
differences from all other strains, while 27 of the outbreak
representatives could be assigned to the appropriate outbreak with
confidence. The majority of the outbreak isolates had none or 2 band
differences from the index profile, although 3 isolates differed by 5-7
bands. The 2 exceptions among the unrelated strains differed by 4 bands,
and 3 phage typing reactions, and were isolated from London and Berlin 3
yr apart, while the 2 exceptions among the outbreak collection had clearly
unique profiles with over 20 band differences from each other and the
outbreak profiles. Cluster anal. using Dice coefficient and UPGMA gave cut-off
values of 75-78% similarity overall for related isolates, while the
closest similarity for unrelated strains was 70%. The results of this
study together with those of the 6 previous reports of PFGE for S.
marcescens (which used either enzymes XbaI or SpeI) confirm that this
technique is of value for this species and that with XbaI at least, most
epidemiol. related strains will only differ by 3-4 bands. However, on
occasion up to 7 band differences can be found within an apparent
outbreak, which may be suggestive of genetic **drift.**

> d ab 7

L5   ANSWER 7 OF 41   CA   COPYRIGHT 2004 ACS on STN
B   Effects of nonlinear dependence **drift** velocity of
      (double-stranded) DNA vs. elec. field strength were investigated. In
      comparatively weak fields, the mol. **drift** velocity is
      proportional to the external elec. field, while in strong fields there is
      addnl. nonlinear component. This effect offers possibilities to
      manipulate the total **drift** velocity at will-the macromols. of
      different size can be made to move in opposite directions in pulsed field
      gel electrophoresis. A new approach for focusing DNA mols. based on
      nonlinear electrophoresis and geometric trapping in elec. fields is
      proposed. The focusing is carried out in an alternating nonuniform elec.
      field, created by using a wedge gel with hyperbolic boundaries. It is
      shown that the fractions separated in such wedge retain their rectilinear
      shape. Gel electrophoresis expts. supported the possibility of a
      pronounced nonlinear focusing of DNA mols. This nonlinear separation technique
      presents encouraging prospects for micromanipulating systems and also for
      preparative isolation of long DNA fragments and development of new separation
      methods for bacterial **fingerprinting.**

> d ti 11-20

L5   ANSWER 11 OF 41   CA   COPYRIGHT 2004 ACS on STN
I   **Fingerprinting** of Helicobacter pylori strains by matrix-assisted
      laser desorption/ionization mass spectrometric analysis

L5   ANSWER 12 OF 41   CA   COPYRIGHT 2004 ACS on STN
I   Variation of multilocus minisatellite DNA **fingerprints** in avian
      populations

L5   ANSWER 13 OF 41   CA   COPYRIGHT 2004 ACS on STN
I   FTIR-spectroscopy in microbial and material analysis

L5   ANSWER 14 OF 41   CA   COPYRIGHT 2004 ACS on STN
I   Development of an optimized sorbent for direct HPTLC-FTIR online coupling

L5   ANSWER 15 OF 41   CA   COPYRIGHT 2004 ACS on STN
I   Channel plate for electrophoretic DNA sequencing

L5   ANSWER 16 OF 41   CA   COPYRIGHT 2004 ACS on STN
I   Application of laser microprobe inductively coupled plasma mass

spectrometry for trace metal **fingerprinting** of native gold

L15   ANSWER 17 OF 41   CA   COPYRIGHT 2004 ACS on STN
TI   Separation of polyester oligomers by gradient high-performance liquid
      chromatography

L15   ANSWER 18 OF 41   CA   COPYRIGHT 2004 ACS on STN
TI   Mid-infrared as a new tool for detecting adulteration in fruit products

L15   ANSWER 19 OF 41   CA   COPYRIGHT 2004 ACS on STN
TI   Rapid analysis of multiple determinands using pyrolysis mass spectrometry
      and supervised learning with artificial neural networks - principles and
      applications

L15   ANSWER 20 OF 41   CA   COPYRIGHT 2004 ACS on STN
TI   FTIR spectroscopy

=> d 13,19 ab

L15   ANSWER 13 OF 41   CA   COPYRIGHT 2004 ACS on STN
AB   The investigation of the development and the properties of biofilms is
      difficult because classical microbiol. does not offer non-destructive
      methods other than microscopical observations. This paper discusses the
      use of different Fourier transform IR spectroscopy (FTIR-spectroscopy)
      techniques as a means to investigate microorganisms in biofilms.
      FTIR-spectroscopy is suitable for the identification of microorganisms and
      presents a new addition to taxonomic and genetic methods. The FTIR anal. of
      bacterial isolates provides **fingerprint** spectra, allowing the
      rapid characterization of microbial strains. Secondly, the
      FTIR-attenuated total reflection (ATR) technique can be used for the
      observation of biofilms forming directly on the interface of an ATR
      crystals such as germanium. These crystals can be coated to obtain a
      surface more relevant to study interfacial processes. Spectra can be
      acquired non-destructively, in situ and in real time. This method is
      suitable for fundamental biofilm research, as well as for monitoring of
      biofilm formation, e.g., in an ultrapure or drinking water systems.
      Furthermore, FTIR-ATR also allows the rapid anal. of deposits on surfaces,
      e.g., filtration membranes. The anal. discrimination between
      microorganisms, inorg. material or other foulants can be obtained.
      Thirdly, with the diffuse reflectance technique (**DRIFT**) it is
      possible to investigate reflecting surfaces like metals or very small
      samples. The composition of surface coatings like biomass or other surface
      contaminants can be detected. These different measurement techniques
      demonstrate that FTIR -spectroscopy is suitable for biofilm and surface
      anal. and can be applied in many different ways.

15   ANSWER 19 OF 41   CA   COPYRIGHT 2004 ACS on STN
AB   Curie-point pyrolysis mass spectrometry is a rapid, high-resolution technique
      which has enjoyed historical success in the operational
      fingerprinting and classification of microbial and other biol.
      systems. More recently we have exploited the anal. power of this
      technique together with supervised learning, based on artificial neural
      networks and cognate chemometric methods, for the accurate and quant.
      anal. of complex biol. materials, including microorganisms, fermentor
      broths and agricultural products. When suitable stds. are available,
      supervised learning is much more powerful than in unsupervised learning
      for the chemometric anal. of multivariate spectroscopic data. Similar
      neural network methods may also be used to correct for mass spectral
      drift.

> d 19

15   ANSWER 19 OF 41   CA   COPYRIGHT 2004 ACS on STN
N   127:106297   CA
I   Rapid analysis of multiple determinands using pyrolysis mass spectrometry
      and supervised learning with artificial neural networks - principles and
      applications